

Towards A Deeper Geometric, Analytic and Algorithmic Understanding of Margins

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Abstract

Given a matrix A , a linear feasibility problem (of which linear classification is a special case) aims to find a solution to a primal problem $w : A^T w > \mathbf{0}$ or a certificate for the dual problem which is a probability distribution $p : Ap = \mathbf{0}$. Inspired by the continued importance of “large-margin classifiers” in machine learning, this paper studies a condition measure of A called its *margin* that determines the difficulty of both the above problems. To aid geometrical intuition, we first establish new characterizations of the margin in terms of relevant balls, cones and hulls. Our second contribution is analytical, where we present generalizations of Gordan’s theorem, and variants of Hoffman’s theorems, both using margins. We end by proving some new results on a classical iterative scheme, the Perceptron, whose convergence rates famously depends on the margin. Our results are relevant for a deeper understanding of margin-based learning and proving convergence rates of iterative schemes, apart from providing a unifying perspective on this vast topic.

1 Introduction

Assume that we have a $d \times n$ matrix A representing n points a_1, \dots, a_n in \mathbb{R}^d . In this paper, we will be concerned with linear feasibility problems that ask if there exists a vector $w \in \mathbb{R}^d$ that makes positive dot-product with every a_i , i.e.

$$\exists w : A^T w > \mathbf{0}, \quad (\text{P})$$

where boldfaced $\mathbf{0}$ is a vector of zeros. The corresponding algorithmic question is “if (P) is feasible, how quickly can we find a w that demonstrates (P)’s feasibility?”.

Such problems abound in optimization as well as machine learning. For example, consider *binary linear classification* - given n points $x_i \in \mathbb{R}^d$ with labels $y_i \in \{+1, -1\}$, a classifier w is said to separate the given points if $w^T x_i$ has the same sign as y_i or succinctly $y_i(w^T x_i) > 0$ for all i . Representing $a_i = y_i x_i$ shows that this problem is a specific instance of (P).

We call (P) the *primal* problem, and (we will later see why) we define the *dual* problem (D) as:

$$? \exists p \geq \mathbf{0} : Ap = \mathbf{0}, p \neq \mathbf{0}, \quad (\text{D})$$

and the corresponding algorithmic question is “if (D) is feasible, how quickly can we find a certificate p that demonstrates feasibility of (D)?”.

Our aim is to deepen the geometric, algebraic and algorithmic understanding of the problems (P) and (D), tied together by a concept called *margin*. Geometrically, we provide intuition about ways to interpret margin in the primal and dual settings relating to various balls, cones and hulls. Analytically, we prove new margin-based versions of classical results in convex analysis like Gordan’s and Hoffman’s theorems. Algorithmically, we give new insights into the classical Perceptron algorithm. We begin with a gentle introduction to some of these concepts, before getting into the details.

Notation When we write $v \geq w$ for vectors v, w , we mean $v_i \geq w_i$ for all their indices i (similarly $v \leq w, v = w$). To distinguish surfaces and interiors of balls more obviously to the eye in mathematical equations, we choose to denote Euclidean balls in \mathbb{R}^d by $\circ := \{w \in \mathbb{R}^d : \|w\| = 1\}$, $\bullet := \{w \in \mathbb{R}^d : \|w\| \leq 1\}$ and the probability simplex \mathbb{R}^n by $\triangle := \{p \in \mathbb{R}^n : p \geq \mathbf{0}, \|p\|_1 = 1\}$. We denote the linear subspace spanned by A as $\text{lin}(A)$, and convex hull of A by $\text{conv}(A)$. Lastly, define $\bullet_A := \bullet \cap \text{lin}(A)$ and $r\bullet$ is the ball of radius r ($\circ_A, r\circ$ are similarly defined).

1.1 Margin ρ

The margin of the problem instance A is classically defined as

$$\begin{aligned} \rho &:= \sup_{w \in \circ} \inf_{p \in \triangle} w^T Ap \\ &= \sup_{w \in \circ} \inf_i w^T a_i. \end{aligned} \quad (1)$$

If there is a w such that $A^T w > \mathbf{0}$, then $\rho > 0$. If for all w , there is a point at an obtuse angle to it, then $\rho < 0$. At the boundary ρ can be zero. The $w \in \circ$ in the definition is important – if it were $w \in \bullet$, then ρ would be non-negative, since $w = 0$ would be allowed.

This definition of margin was introduced by Goffin [13] who gave several geometric interpretations. It has since been extensively studied (for example, [20, 21] and [4]) as a notion of complexity and conditioning of a problem instance. Broadly, the larger its magnitude, the better conditioned the pair of feasibility problems (P) and (D) are, and the easier it is to find witnesses of their feasibility. Ever since [25], the margin-based algorithms have been extremely popular with a growing literature in machine learning which it is not relevant to presently summarize.

In Sec. 2, we define an important and “corrected” variant of the margin, which we call *affine-margin*, that turns out to be the actual quantity determining convergence rates of iterative algorithms.

Gordan’s Theorem This is a classical *theorem of the alternative*, see [3, 5]. It implies that exactly one of (P) and (D) is feasible. Specifically, it states that exactly one of the following statements is true.

1. There exists a w such that $A^T w > \mathbf{0}$.
2. There exists a $p \in \Delta$ such that $Ap = \mathbf{0}$.

This, and other separation theorems like Farkas’ Lemma (see above references), are widely applied in algorithm design and analysis. We will later prove generalizations of Gordan’s theorem using affine-margins.

Hoffman’s Theorem The classical version of the theorem from [15] characterizes how close a point is to the solution set of the feasibility problem $Ax \leq b$ in terms of the amount of violation in the inequalities and a problem dependent constant. In a nutshell, if $\mathbb{S} := \{x | Ax \leq b\} \neq \emptyset$ then

$$\text{dist}(x, \mathbb{S}) \leq \tau \| [Ax - b]_+ \| \quad (2)$$

where τ is the “Hoffman constant” and it depends on A but is *independent of b* . This and similar theorems have found extensive use in convergence analysis of algorithms - examples include [12, 16, 23].

Güler, Hoffman, and Rothblum [14] generalize this bound to any norms on the left and right hand sides of the above inequality. We will later prove theorems of a similar flavor for (P) and (D), where τ^{-1} will almost magically turn out to be the affine-margin. Such theorems are used for proving rates of convergence of algorithms, and having the constant explicitly in terms of a familiar quantity is useful.

1.2 Summary of Contributions

- **Geometric:** In Sec.2, we define the *affine-margin*, and argue why a subtle difference from Eq.(1) makes it the “right” quantity to consider, especially for problem (D). We then establish geometrical characterizations of the affine-margin when (P) is feasible as well as when (D) is feasible and connect it to well-known *radius theorems*. This is the paper’s appetizer.
- **Analytic:** Using the preceding geometrical insights, in Sec.3 we prove two generalizations of Gordan’s Theorem to deal with alternatives involving the affine-margin when either (P) or (D) is strictly feasible. Building on this intuition further, in Sec.4, we prove several interesting variants of Hoffman’s Theorem, which explicitly involve the affine-margin when either (P) or (D) is strictly feasible. This is the paper’s main course.
- **Algorithmic:** In Sec.5, we prove new properties of the Normalized Perceptron, like its margin-maximizing and margin-approximating property for (P) and dual convergence for (D). This is the paper’s dessert.

We end with a historical discussion relating Von-Neumann’s and Gilbert’s algorithms, and their advantage over the Perceptron.

2 From Margins to *Affine*-Margins

An important but subtle point about margins is that the quantity determining the difficulty of solving (P) and (D) is actually *not* the margin as defined classically in Eq.(1), but the affine-margin which is the margin when w is restricted to $\text{lin}(A)$, i.e. $w = A\alpha$ for some coefficient vector $\alpha \in \mathbb{R}^n$. The affine-margin is defined as

$$\begin{aligned}\rho_A &:= \sup_{w \in \bigcirc_A} \inf_{p \in \Delta} w^T A p \\ &= \sup_{\|\alpha\|_G=1} \inf_{p \in \Delta} \alpha^T G p\end{aligned}\tag{3}$$

where $G = A^T A$ is a key quantity called the Gram matrix, and $\|\alpha\|_G = \sqrt{\alpha^T G \alpha}$ is easily seen to be a self-dual semi-norm.

Intuitively, when the problem (P) is infeasible but A is not full rank, i.e. $\text{lin}(A)$ is not \mathbb{R}^d , then ρ will never be negative (it will always be zero), because one can always pick w as a unit vector perpendicular to $\text{lin}(A)$, leading to a zero dot-product with every a_i . Since no matter how easily inseparable A is, the margin is always zero if A is low rank, this definition does not capture the difficulty of verifying linear infeasibility.

Similarly, when the problem (P) is feasible, it is easy to see that searching for w in directions perpendicular to A is futile, and one can restrict attention to $\text{lin}(A)$, again making this the right quantity in some sense. For clarity, we will refer to

$$\rho_A^+ := \max\{0, \rho_A\} \quad ; \quad \rho_A^- := \min\{0, \rho_A\}\tag{4}$$

when the problem (P) is strictly feasible ($\rho_A > 0$) or strictly infeasible ($\rho_A < 0$) respectively.

We remark that when $\rho > 0$, we have $\rho_A^+ = \rho_A = \rho$, so the distinction really matters when $\rho_A < 0$, but it is still useful to make it explicit. One may think that if A is not full rank, performing PCA would get rid of the unnecessary dimensions. However, we often wish to only perform elementary operations on (possibly large matrices) A that are much simpler than eigenvector computations.

Instability of ρ_A^- compared to ρ

Unfortunately, the behaviour of ρ_A^- is quite finicky – unlike ρ_A^+ it is not stable to small perturbations when $\text{conv}(A)$ is not full-dimensional. To be more specific, if (P) is strictly feasible and we perturb all the vectors by a small amount or add a vector that maintains feasibility, ρ_A^+ can only change by a small amount. However, if (P) is strictly *infeasible* and we perturb all the vectors by a small amount or add a vector that maintains infeasibility, ρ_A^- can change by a large amount.

For example, assume $\text{lin}(A)$ is not full-dimensional, and $|\rho_A^-|$ is large. If we add a new vector v to A to form $A' = \{A \cup v\}$ where v has a even a tiny component v^\perp orthogonal to $\text{lin}(A)$, then $\rho_{A'}^-$ suddenly becomes zero. This is because it is now possible to choose a vector $w = v^\perp / \|v^\perp\|$ which is in $\text{lin}(A')$, and makes zero dot-product with A , and positive dot-product with v . Similarly, instead of adding a vector, if we perturb a given set of vectors so that $\text{lin}(A)$ increases dimension, the negative margin can suddenly jump from to zero.

Despite its instability and lack of “continuity”, it is indeed this negative affine margin that determines rate of convergence of algorithms for (D). In particular, the convergence rate of the von Neumann–Gilbert algorithm for (D) is determined by ρ_A^- much the same way as the convergence rate of the perceptron algorithm for (P) is determined by ρ_A^+ . We discuss these issues in detail in Section 5 and Section 6.1.

2.1 Geometric Interpretations of ρ_A^+

The positive margin has many known geometric interpretations – it is the width of the feasibility cone, and also the largest ball centered on the unit sphere that can fit inside the dual cone ($w : A^T w > \mathbf{0}$ is the dual cone of $\text{cone}(A)$) – see, for example [4, 10]. Here, we provide a few more interpretations. Remember that $\rho_A^+ = \rho$ when Eq.(P) is feasible.

Proposition 1. *The distance of the origin to $\text{conv}(A)$ is ρ_A^+ .*

$$\rho_A^+ = \inf_{p \in \Delta} \|p\|_G = \inf_{p \in \Delta} \|Ap\| \quad (5)$$

Proof. When $\rho_A \leq 0$, $\rho_A^+ = 0$ and Eq.(5) holds because (D) is feasible making the right hand side also zero. When $\rho_A > 0$,

$$\rho_A^+ = \sup_{w \in \bigcirc} \inf_{p \in \Delta} w^T Ap = \sup_{w \in \bullet} \inf_{p \in \Delta} w^T Ap = \inf_{p \in \Delta} \sup_{w \in \bullet} w^T Ap = \inf_{p \in \Delta} \|Ap\|. \quad (6)$$

Note that the first two equalities holds when $\rho_A > 0$, the next by the minimax theorem, and the last by self-duality of $\|\cdot\|$. \square

The quantity ρ_A^+ is also closely related to a particular instance of the Minimum Enclosing Ball (MEB) problem. While it is common knowledge that MEB is connected to margins (and support vector machines), it is possible to explicitly characterize this relationship, as we have done below.

Proposition 2. *Assume $A = [a_1 \ \cdots \ a_n] \in \mathbb{R}^{d \times n}$ and $\|a_i\| = 1$, $i = 1, \dots, n$. Then the radius of the minimum enclosing ball of $\text{conv}(A)$ is $\sqrt{1 - \rho_A^{+2}}$.*

Proof. It is a simple exercise to show that the following are the MEB problem, and its Lagrangian dual

$$\begin{aligned} \min_{c, r} \quad & r^2 \quad \text{s.t.} \quad \|c - a_i\|^2 \leq r^2 \\ \max_{p \in \Delta} \quad & 1 - \|Ap\|^2. \end{aligned} \quad (7)$$

The result then follows from Proposition 1. \square

As we show in Section 5, the (Normalized) Perceptron and related algorithms that we introduce later yields a sequence of iterates that converge to the center of the MEB, and if the distance of the origin to $\text{conv}(A)$ is zero (because $\rho_A < 0$), then the sequence of iterates converges to the origin, and the MEB just ends up being the unit ball.

2.2 Geometric Interpretations of $|\rho_A^-|$

Proposition 3. *If $\rho_A \leq 0$ then $|\rho_A^-|$ is the radius of the largest Euclidean ball centered at the origin that completely fits inside the relative interior of the convex hull of A . Mathematically,*

$$|\rho_A^-| = \sup \left\{ R \mid \|\alpha\|_G \leq R \Rightarrow A\alpha \in \text{conv}(A) \right\}. \quad (8)$$

Proof. We split the proof into two parts, one for each inequality.

(1) For inequality \geq . Choose any R such that $A\alpha \in \text{conv}(A)$ for any $\|\alpha\|_G \leq R$. Given an arbitrary $\|\alpha'\|_G = 1$, put $\tilde{\alpha} := -R\alpha'$. By our assumption on R , since $\|\tilde{\alpha}\|_G = R$, we can infer that $A\tilde{\alpha} \in \text{conv}(A)$ implying there exists a $\tilde{p} \in \Delta$ such that $A\tilde{\alpha} = A\tilde{p}$. Also

$$\alpha'^T G \tilde{p} = \alpha'^T G \tilde{\alpha} = -R \|\alpha'\|_G^2 = -R.$$

Thus $\inf_{p \in \Delta} \alpha'^T G p \leq -R$. Since this holds for any $\|\alpha'\|_G = 1$, it follows that

$$\sup_{\|\alpha\|_G=1} \inf_{p \in \Delta} \alpha^T G p \leq -R.$$

In other words, $|\rho_A^-| \geq R$.

(2) For inequality \leq . It suffices to show $\|\alpha\|_G \leq |\rho_A^-| \Rightarrow A\alpha \in \text{conv}(A)$. We will prove the contrapositive $A\alpha \notin \text{conv}(A) \Rightarrow \|\alpha\|_G > |\rho_A^-|$. Since $\text{conv}(A)$ is closed and convex, if $A\alpha \notin \text{conv}(A)$, then there exists a hyperplane separating $A\alpha$ and $\text{conv}(A)$ in $\text{lin}(A)$. That is, there exists (β, b) with $\|A\beta\| = 1$ in $\text{lin}(A)$ and a constant $b \in \mathbb{R}$ such that $\beta^T A^T A \alpha = \beta^T G \alpha < b$ and $\beta^T A^T A p = \beta^T G p \geq b$ for all $p \in \Delta$. In particular,

$$\beta^T G \alpha < \inf_{p \in \Delta} \beta^T G p \leq \sup_{\|\beta\|_G=1} \inf_{p \in \Delta} \beta^T G p = \rho_A^-.$$

Since $\rho_A^- \leq 0$, it follows that $|\rho_A^-| < |\beta^T G \alpha| \leq \|\beta\|_G \|\alpha\|_G = \|\alpha\|_G$. □

One might be tempted to deal with the usual margin and prove that

$$|\rho| = \sup \left\{ R \mid \|w\| \leq R \Rightarrow w \in \text{conv}(A) \right\} \quad (9)$$

While the two definitions are equivalent for full-dimensional $\text{lin}(A)$, they differ when $\text{lin}(A)$ is not full-dimensional, which is especially relevant in the context of infinite dimensional reproducing kernel Hilbert spaces, but could even occur when A is low rank. In this case, Eq.(9) will always be zero since a full-dimensional ball cannot fit inside a finite-dimensional hull. The right thing to do is to only consider balls ($\|\alpha\|_G \leq R$) in the linear subspace spanned by columns of A (or the relative interior of the convex hull of A) and not full-dimensional balls ($\|w\| \leq R$). The reason it matters is that it is this altered $|\rho_A^-|$ that determines rates for algorithms and the complexity of problem (D), and not the classical margin in Eq.(1) as one might have expected.

“Radius Theorems”

Recall that $A\Delta = \{Ap : p \in \Delta\} = \text{conv}(A)$, $\bullet_A = \bullet \cap \text{lin}(A)$, and $R\bullet_A$ is just \bullet_A of radius R . Since $\|\alpha\|_G \leq R \Leftrightarrow \|A\alpha\| \leq R \Leftrightarrow A\alpha \in R\bullet_A$, an enlightening restatement of Eq.(8) and Eq.(9) is

$$|\rho_A^-| = \sup \left\{ R \mid R\bullet_A \subseteq A\Delta \right\}, \text{ and } |\rho| = \sup \left\{ R \mid R\bullet \subseteq A\Delta \right\}.$$

It can be read as “largest radius (affine) ball that fits inside the convex hull”. There is a nice parallel to the smallest (overall) and smallest positive singular values of a matrix. Using $A\bullet = \{Ax : x \in \bullet\}$ for brevity,

$$\sigma_{\min}^+(A) = \sup \left\{ R \mid R\bullet_A \subseteq A\bullet \right\}, \text{ and } \sigma_{\min}(A) = \sup \left\{ R \mid R\bullet \subseteq A\bullet \right\} \quad (10)$$

This highlights the role of the margin is a measure of conditioning of the linear feasibility systems (P) and (D). Indeed, there are a number of far-reaching extensions of the classical “radius theorem” of [7]. The latter states that the Euclidean distance from a square non-singular matrix $A \in \mathbb{R}^{n \times n}$ to the set of singular matrices in $\mathbb{R}^{n \times n}$ is precisely $\sigma_{\min}(A)$. In an analogous fashion, for the feasibility problems (P) and (D), the set Σ of *ill-posed* matrices A are those with $\rho = 0$. Cheung and Cucker [4] show that for a given a matrix $A \in \mathbb{R}^{m \times n}$ with normalized columns, the margin is the largest perturbation of a row to get an ill-posed instance or the “distance to ill-posedness”, i.e.

$$\min_{\tilde{A} \in \Sigma} \max_{i=1, \dots, n} \|a_i - \tilde{a}_i\| = |\rho|. \quad (11)$$

See [4, 21] for related discussions.

3 Gordan’s Theorem with Margins

We would like to make quantitative statements about what happens when either of the alternatives is satisfied *easily* (with large positive or negative margin). Our preceding geometrical intuition suggests a refinement of Gordan’s Theorem, namely Theorem 1 below, that accounts for margins. Related results have been previously derived and discussed by Li and Terlaky [17] as well as by Todd and Ye [24]. In particular, it can be shown that part 2 of Theorem 1 could be obtained from [24, Lemma 2.1 and Lemma 2.2]. Similarly, parts 2 and 3 could be recovered from [17, Theorem 5 and Theorem 6]. We give a succinct and simple proof of Theorem 1 by relying on Proposition 1 and Proposition 3. Theorem 1 could also be proven, albeit less succinctly, via separation arguments from convex analysis.

Theorem 1. *For any problem instance A and any constant $\gamma \geq 0$,*

1. *Either $\exists w \in \circ_A$ s.t. $A^T w > \mathbf{0}$, or $\exists p \in \Delta$ s.t. $Ap = \mathbf{0}$.*
2. *Either $\exists w \in \circ_A$ s.t. $A^T w > \gamma \mathbf{1}$, or $\exists p \in \Delta$ s.t. $\|Ap\| \leq \gamma$.*
3. *Either $\exists w \in \circ_A$ s.t. $A^T w > -\gamma \mathbf{1}$, or $\forall v \in \gamma\bullet_A \exists p_v \in \Delta$ s.t. $v = Ap_v$.*

Proof. The first statement is the usual form of Gordan's Theorem. It is also a particular case of the other two when $\gamma = 0$. Thus, we will prove the other two:

2. If the first alternative does not hold, then from the definition of ρ_A it follows that $\rho_A \leq \gamma$. In particular, $\rho_A^+ \leq \gamma$. To finish, observe that by Proposition 1 there exists $p \in \Delta$ such that

$$\|Ap\| = \rho_A^+ \leq \gamma. \quad (12)$$

3. Analogously to the previous case, if the first alternative does not hold, then $\rho_A \leq -\gamma$. In particular, it captures

$$|\rho_A^-| \geq \gamma. \quad (13)$$

Observe that by Proposition 3, every point $v \in \gamma \bullet_A$ must be inside $\text{conv}(A)$, that is, $v = Ap_v$ for some distribution $p_v \in \Delta$.

One can similarly argue that in each case if the first alternative is true, then the second must be false. \square

In the spirit of radius theorems introduced in the previous section, the statements in Theorem 1 can be equivalently written in the following succinct forms:

- 1'. Either $\{w \in \circ_A : A^T w > \mathbf{0}\} \neq \emptyset$, or $\mathbf{0} \in A\Delta$
- 2'. Either $\{w \in \circ_A : A^T w > \gamma \mathbf{1}\} \neq \emptyset$, or $\gamma \bullet_A \cap A\Delta \neq \emptyset$
- 3'. Either $\{w \in \circ_A : A^T w > -\gamma \mathbf{1}\} \neq \emptyset$, or $\gamma \bullet_A \subseteq A\Delta$

As noted in the proof of Theorem 1, the first statement is a special case of the other two when $\gamma = 0$. In case 2, we have at least one witness p close to the origin, and in 3, we have an entire ball of witnesses close to the origin.

4 Hoffman's Theorem with Margins

Hoffman-style theorems are often useful to prove the convergence rate of iterative algorithms by characterizing the distance of a current iterate from a target set. For example, a Hoffman-like theorem was also proved by [16] (Lemma 2.3), where they use it to prove the linear convergence rate of the alternating direction method of multipliers, and in [12] (Lemma 4), where they use it to prove the linear convergence of a first order algorithm for calculating ϵ -approximate equilibria in zero sum games.

It is worth pointing out that Hoffman, in whose honor the theorem is named and also an author of [14] whose proof strategy we follow in the alternate proof of Theorem 3, himself appeared to have overlooked the intimate connection of the ‘‘Hoffman constant’’ (τ in Eq.(2)) to the positive and negative margin, as we present in our theorems below.

4.1 Hoffman's theorem for (D) when $\rho_A^- \neq 0$

Theorem 2. Assume $A \in \mathbb{R}^{m \times n}$ is such that $|\rho_A^-| > 0$. For $b \in \mathbb{R}^m$ define the “witness” set $W = \{x \geq \mathbf{0} | Ax = b\}$. If $W \neq \emptyset$ then for all $x \geq \mathbf{0}$,

$$\text{dist}_1(x, W) \leq \frac{\|Ax - b\|}{|\rho_A^-|} \quad (14)$$

where $\text{dist}_1(x, W)$ is the distance from x to W measured by the ℓ_1 norm $\|\cdot\|_1$.

Proof. Given $x \geq \mathbf{0}$ with $Ax \neq b$, consider a point

$$v = |\rho_A^-| \frac{b - Ax}{\|Ax - b\|} \quad (15)$$

Note that $\|v\| = |\rho_A^-|$ and crucially $v \in \text{lin}(A)$ (since $b \in \text{lin}(A)$ since $W \neq \emptyset$). Hence, by Theorem 1, there exists a distribution p such that $v = Ap$. Define

$$\bar{x} = x + p \frac{\|Ax - b\|}{|\rho_A^-|} \quad (16)$$

Then, by substitution for p and v one can see that

$$A\bar{x} = Ax + v \frac{\|Ax - b\|}{|\rho_A^-|} = Ax + (b - Ax) = b \quad (17)$$

Hence $\bar{x} \in W$, and $\text{dist}_1(x, W) \leq \|x - \bar{x}\|_1 = \frac{\|Ax - b\|}{|\rho_A^-|}$. \square

The following variation (using witnesses only in Δ) on the above theorem also holds. This result is closely related to [23, Lemma 2] and has essentially the same proof.

Proposition 4. Assume $A \in \mathbb{R}^{m \times n}$ is such that $|\rho_A^-| > 0$. Define the set of witnesses $W = \{p \in \Delta | Ap = \mathbf{0}\}$. Then at any $p \in \Delta$,

$$\text{dist}_1(p, W) \leq \frac{2\|Ap\|}{\|Ap\| + |\rho_A^-|} \leq \frac{2\|Ap\|}{|\rho_A^-|} = \frac{2\|p\|_G}{|\rho_A^-|}. \quad (18)$$

Proof. Assume $Ap \neq 0$ as otherwise there is nothing to show. Consider $v := -\frac{|\rho_A^-|}{\|Ap\|} Ap$. Since $v \in \text{lin}(A)$ and $\|v\| = |\rho_A^-|$, Proposition 3 implies that $v = Ap'$ for some $p' \in \Delta$. Thus for $\lambda := \frac{\|Ap\|}{\|Ap\| + |\rho_A^-|}$ we have $\tilde{p} := \lambda p' + (1 - \lambda)p \in W$ and

$$\text{dist}_1(p, W) \leq \|p - \tilde{p}\|_1 = \lambda \|p - p'\|_1 \leq 2\lambda = \frac{2\|Ap\|}{\|Ap\| + |\rho_A^-|} = \frac{2\|Ap\|}{|\rho_A^-|} = \frac{2\|p\|_G}{|\rho_A^-|}.$$

\square

4.2 Hoffman's theorem for (P) when $\rho_A^+ \neq 0$

Theorem 3. Define $S = \{y | A^T y \geq c\}$ for some vector c . Then, for all $w \in \mathbb{R}^d$,

$$\text{dist}(w, S) \leq \frac{\|[A^T w - c]^-\|_\infty}{\rho_A^+}$$

where $\text{dist}(w, S)$ is the $\|\cdot\|_2$ -distance from w to S and $(x^-)_i = \min\{x_i, 0\}$.

Proof. Since $\rho_A^+ > 0$, the definitions of margin (1) and affine margin (3) imply that there exists $\bar{w} \in \circ_A$ with $A^T \bar{w} \geq \rho_A^+ \mathbf{1}$. Suppose, $A^T w \not\geq c$. Then we can add a multiple of \bar{w} to w as follows. Let $a = [c - A^T w]^+ = -[A^T w - c]^-$ where $(x^+)_i = \max\{x_i, 0\}$ and $(x^-)_i = \min\{x_i, 0\}$. Since $a \geq c - A^T w$ and $a \geq 0$, we have $\|a\|_\infty \mathbf{1} \geq c - A^T w$ and consequently

$$A^T \left(w + \frac{\|a\|_\infty}{\rho_A^+} \bar{w} \right) \geq A^T w + \|a\|_\infty \mathbf{1} \geq A^T w + (c - A^T w) = c.$$

Hence, $w + \frac{\|a\|_\infty}{\rho_A^+} \bar{w} \in S$ whose distance from w is precisely $\frac{\|a\|_\infty}{\rho_A^+}$. \square

The interpretation of the preceding theorem is that the distance to feasibility for the problem (P) is governed by the magnitude of the largest mistake and the positive affine-margin of the problem instance A .

We also provide an alternative proof of the theorem above, since proving the same fact from completely different angles can often yield insights. We follow the techniques of [14], though we significantly simplify it. This is perhaps a more classical proof style, and possibly more amenable to other bounds not involving the margin, and hence it is instructive for those unfamiliar with proving these sorts of bounds.

Alternate Proof of Theorem 3. For any given w , define $a = -(A^T w - c)^- = (-A^T w + c)^+$ and hence note that $a \geq -(A^T w - c)$.

$$\begin{aligned} \min_{A^T u \geq c} \|w - u\| &= \min_{A^T(u-w) \geq -A^T w + c} \|w - u\| = \min_{A^T z \geq -A^T w + c} \|z\| \\ &= \sup_{\|\mu\| \leq 1} \left(\min_{A^T z \geq -A^T w + c} \mu^T z \right) \end{aligned} \quad (19)$$

$$= \sup_{\|\mu\| \leq 1} \left(\sup_{p \geq \mathbf{0}, Ap = \mu} p^T (-A^T w + c) \right) \quad (20)$$

$$= \sup_{\|p\|_G \leq 1, p \geq \mathbf{0}} p^T (-A^T w + c) \quad (21)$$

$$\begin{aligned} &\leq \sup_{\|p\|_G \leq 1, p \geq \mathbf{0}} p^T a \leq \sup_{\|p\|_G \leq 1, p \geq \mathbf{0}} \|p\|_1 \|a\|_\infty \\ &= \frac{\|a\|_\infty}{\rho_A^+} \end{aligned} \quad (22)$$

We used the self-duality of $\|\cdot\|$ in Eq.(19), LP duality for Eq.(20), $\|Ap\| = \|p\|_G$ by definition for Eq.(21), and Holder's inequality in Eq.(22). The last equality follows because $\frac{1}{\rho_A^+} = \max_{\|p\|_G=1, p \geq \mathbf{0}} \|p\|_1$, since $\rho_A^+ = \inf_{p \geq \mathbf{0}, \|p\|_1=1} \|p\|_G$ by Proposition 1. \square

5 The Perceptron Algorithm: New Insights

The Perceptron Algorithm was introduced and analysed by [2, 18, 22] to solve the primal problem (P), with many variants in the machine learning literature. For ease of notation throughout this section assume $A = [a_1 \cdots a_n] \in \mathbb{R}^{d \times n}$ and $\|a_i\| = 1$, $i = 1, \dots, d$. The classical algorithm starts with $w_0 := a_i$ for any i , and in iteration t performs

$$\begin{aligned} \text{(choose any mistake)} \quad & a_i : w_{t-1}^T a_i \leq 0. \\ & w_t \leftarrow w_{t-1} + a_i. \end{aligned}$$

A variant called Normalized Perceptron which, as we point out in Theorem 4 below, is a subgradient method, only updates on the worst mistake, and tracks a normalized w that which is a convex combination of a_i 's.

$$\begin{aligned} \text{(choose the worst mistake)} \quad & a_i = \arg \min_{a_i} \{w_{t-1}^T a_i\} \\ & w_t \leftarrow \left(1 - \frac{1}{t}\right) w_{t-1} + \left(\frac{1}{t}\right) a_i. \end{aligned}$$

The best known property of the unnormalized Perceptron or the Normalized Perceptron algorithm is that when (P) is strictly feasible with margin ρ_A^+ , it finds such a solution w in $1/\rho_A^{+2}$ iterations, as proved by [18, 2]. What is less obvious is that the Perceptron is actually *primal-dual* in nature, as stated in the following result of Li and Terlaky [17]. In the following statement by an ϵ -certificate for (D) we mean a vector $\alpha \in \Delta$ such that $\|A\alpha\| \leq \epsilon$.

Proposition 5. *If (D) is feasible, the Perceptron algorithm (when normalized) yields an ϵ -certificate α_t for (D) in $1/\epsilon^2$ steps.*

Proposition 5 and Proposition 4 readily yield the following result.

Corollary 1. *Assume (D) is feasible and $|\rho_A^-| > 0$. Define the set of witnesses $W = \{\alpha \in \Delta \mid A\alpha = 0\}$. If $w_t = A\alpha_t$ is the sequence of NP iterates then*

$$\text{dist}_1(\alpha_t, W) \leq \frac{2}{|\rho_A^-| \sqrt{t}}$$

We prove two more nontrivial facts about the Normalized Perceptron that we have not found in the published literature for the case when (P) is feasible. In this case not only does the Normalized Perceptron produce a *feasible* w in $O(1/\rho_A^{+2})$ steps, but on continuing to run the algorithm, w_t will approach the *optimal* w that maximizes margin, i.e., achieves margin ρ_A^+ . This is actually *not* true with the classical Perceptron. The normalization in the following theorem is needed because $\|w_t\| \neq 1$.

Theorem 4. *Assume (P) is feasible. If $w_t = A\alpha_t$, $t = 0, 1, \dots$ is the sequence of NP iterates with margin $\rho_t = \inf_{p \in \Delta} \frac{w_t^T p}{\|w_t\|}$, and the optimal point $w^* := \arg \sup_{\|w\|=1} \inf_{p \in \Delta} w^T p$ achieves the optimal margin $\rho = \rho_A^+ = \sup_{w \in \Delta} \inf_{p \in \Delta} w^T p$, then*

$$\rho_A^+ - \rho_t \leq \left\| \frac{w_t}{\|w_t\|} - w^* \right\| \leq \frac{4}{\rho_A^+ \sqrt{t}}.$$

Proof. Let $p_t := \arg \min_{p \in \Delta} w_t^T A p$. Then

$$\rho_A^+ - \rho_t = \inf_{p \in \Delta} w_t^T A p - \frac{w_t^T}{\|w_t\|} A p_t \leq \left(w_* - \frac{w_t}{\|w_t\|} \right)^T A p_t \leq \left\| \frac{w_t}{\|w_t\|} - w_* \right\| \|A p_t\| \leq \left\| \frac{w_t}{\|w_t\|} - w_* \right\|.$$

The last step because $\|a_i\| = 1$, $i = 1, \dots, n$ and $p \in \Delta$.

For the second inequality, first observe that

$$\begin{aligned} \left\| \frac{w_t}{\|w_t\|} - w_* \right\| &= \frac{1}{\|w_t\|} \left\| w_t - \rho_A^+ w_* + (\rho_A^+ - \|w_t\|) w_* \right\| \\ &\leq \frac{1}{\|w_t\|} \left(\|w_t - \rho_A^+ w_*\| + |\rho_A^+ - \|w_t\|| \right) \\ &\leq \frac{1}{\rho_A^+} \left(\|w_t - \rho_A^+ w_*\| + |\rho_A^+ - \|w_t\|| \right) \end{aligned} \quad (23)$$

where the first inequality follows by the triangle inequality, and because $\|w_*\| = 1$. The second inequality holds because $\rho_A^+ = \inf_{p \in \Delta} \|A p\|$ and $\alpha_t \in \Delta$ implies that

$$\|w_t\| = \|A \alpha_t\| \geq \rho_A^+. \quad (24)$$

The rest of the proof hinges on the fact that NP can be interpreted as a subgradient algorithm for the following problem:

$$\min_{w \in \mathbb{R}^m} L(w) := \min_{w \in \mathbb{R}^m} \left(\frac{1}{2} \|w\|^2 - \min_i \{w^T a_i\} \right). \quad (25)$$

We reproduce a short argument from [19, 23] which shows that $L(w)$ is minimized at $\rho_A^+ w_*$. Let $\arg \min_{\alpha} L(w) = t w'$ for some $\|w'\| = 1$ and some $t \in \mathbb{R}$. Substituting this into Eq.(25), we see that

$$\min_{w \in \mathbb{R}^m} L(w) = \min_{t > 0} \left\{ \frac{1}{2} t^2 - t \rho_A^+ \right\} = -\frac{1}{2} \rho_A^{+2}$$

achieved at $t = \rho_A^+$ and $w' = w_*$. Hence $\arg \min_w L(w) = \rho_A^+ w_*$.

Note that the $(t + 1)$ -th iteration in the NP algorithm can be written as

$$w_{t+1} = w_t - \frac{1}{t+1} g_t,$$

for $g_t = w_t - \arg \min_{a_i} \{w_t^T a_i\} \in \partial L(w_t)$. Hence, the NP algorithm is a subgradient method for (25). By construction, $L(w)$ is a 1-strongly convex function. Since it is minimized at $\rho_A^+ w_*$, it follows that

$$g_t^T (w_t - \rho_A^+ w_*) \geq L(w_t) - L(\rho_A^+ w_*) + \frac{1}{2} \|w_t - \rho_A^+ w_*\|^2 \geq \|w_t - \rho_A^+ w_*\|^2.$$

In addition, $\|g_t\| \leq \|w_t\| (1 + \|a_i\|) \leq 2 \|A \alpha_t\| \leq 2$, so

$$\begin{aligned} \|w_{t+1} - \rho_A^+ w_*\|^2 &= \left\| w_t - \frac{1}{t+1} g_t - \rho_A^+ w_* \right\|^2 \\ &= \|w_t - \rho_A^+ w_*\|^2 - \frac{2}{t+1} g_t^T (w_t - \rho_A^+ w_*) + \frac{1}{(t+1)^2} \|g_t\|^2 \\ &\leq \left(1 - \frac{2}{t+1} \right) \|w_t - \rho_A^+ w_*\|^2 + \frac{4}{(t+1)^2}. \end{aligned}$$

It thus follows by induction on t that

$$\begin{aligned} \|w_t - \rho_A^+ w_*\| &\leq 2/\sqrt{t} \\ \Rightarrow \|w_t\| - \rho_A^+ &\leq 2/\sqrt{t}. \end{aligned} \tag{26}$$

This yields the required bound of $\frac{4}{\rho_A^+ \sqrt{t}}$ when plugged into Eq.(23). \square

Let us revisit the primal-dual formulation (7) of the minimum enclosing ball problem. The center of the minimum enclosing ball is precisely $c_* = \rho_A^+ w_*$. Consequently the following result readily follows.

Corollary 2. *The sequence $w_t = A\alpha_t$, $t = 0, 1, \dots$ of NP iterates converges to the center $c_* = \rho_A^+ w_*$ of the minimum enclosing ball problem (7).*

The Normalized Perceptron algorithm also gives for free an estimate of ρ_A^+ .

Proposition 6. *The Normalized Perceptron gives an ϵ -approximation to the value of the positive margin in $4/\epsilon^2$ steps. Specifically,*

$$\|w_{4/\epsilon^2}\| - \epsilon \leq \rho_A^+ \leq \|w_{4/\epsilon^2}\|$$

Proof. The proof follows from Eq.(26) and Eq.(24), which imply that w_t satisfies

$$\rho_A^+ \leq \|w_t\| \leq \rho_A^+ + 2/\sqrt{t}$$

whose rearrangement with $t = 4/\epsilon^2$ completes the proof. \square

It is worth noting that in sharp contrast to the estimate on ρ_A^+ given by Proposition 6, the question of finding elementary algorithms to estimate $|\rho_A^-|$ remains open.

6 Discussion

6.1 Von-Neumann or Gilbert Algorithm for (D)

Von-Neumann described an iterative algorithm for solving dual (D) in a private communication with Dantzig in 1948, which was subsequently analyzed by the latter, but only published in [6], and goes by the name of Von-Neumann's algorithm in optimization circles. Independently, Gilbert [11] described an essentially identical algorithm that goes by the name of Gilbert's algorithm in the computational geometry literature. We respect the independent findings in different literatures, and refer to it as the Von-Neumann-Gilbert (VNG) algorithm. It starts from a point in $\text{conv}(A)$, say $w := a_1$ and loops:

$$\begin{aligned} \text{(choose furthest point)} \quad & a_i = \arg \max_{a_i} \{\|w_{t-1} - a_i\|\} \\ \text{(line search, } \lambda \in [0, 1]) \quad & w_t \leftarrow \arg \min_{w_\lambda} \|w_\lambda\|; \quad w_\lambda = \lambda w_{t-1} + (1 - \lambda)a_i \end{aligned}$$

Dantzig's paper showed that the Von-Neumann-Gilbert (VNG) algorithm can produce an ϵ -approximate solution (p such that $\|Ap\| \leq \epsilon$) to (D) in $1/\epsilon^2$ steps, establishing it as a

dual algorithm as conjectured by Von-Neumann. Though designed for (D), Epelman and Freund [8] proved that when (P) is feasible, VNG also produces a feasible w in $1/\rho_A^{+2}$ steps and hence VNG is also primal-dual like the Perceptron (as proved in Proposition 5). It readily follows that Theorem 4, Corollary 1, Corollary 2, and Proposition 6 hold as well with the Von-Neumann-Gilbert algorithm in place of the Normalized Perceptron algorithm.

Nesterov was the first to point out in a private note to [9] that VNG is a Frank-Wolfe algorithm for

$$\min_{p \in \Delta} \|Ap\| \quad (27)$$

Note that Eq.(25) is a relaxed version of Eq.(3), and also that Eq.(27) and Eq.(3) are Lagrangian duals of each other as seen in Eq.(6). In this light, it is not surprising that NP and VNG algorithms have such similar properties. Moreover, Bach [1] recently pointed out the strong connection via duality between subgradient and Frank-Wolfe methods.

However, VNG possesses one additional property. Restating a result of [8] – if $|\rho_A^-| > 0$, then VNG has linear convergence. We include a simple geometrical proof of this result.

Proposition 7. *Assume (D) is feasible, $A = [a_1 \ \cdots \ a_n] \in \mathbb{R}^{d \times n}$ with $\|a_i\| = 1$, $i = 1, \dots, d$, and $|\rho_A^-| > 0$. Then the iterates $w_t = A\alpha_t$ generated by the VNG algorithm satisfy*

$$\|w_{t+1}\| \leq \|w_t\| \sqrt{1 - |\rho_A^-|^2}, \quad t = 0, 1, \dots$$

In particular, the algorithm finds $w_t = A\alpha_t$, $\alpha_t \in \Delta$ with $\|w_t\| \leq \epsilon$ in at most $O\left(\frac{1}{|\rho_A^-|^2} \log\left(\frac{1}{\epsilon}\right)\right)$ steps.

Proof. Figure 1 illustrates the idea of the proof. Assume $w_t = A\alpha_t \in \text{lin}(A) \neq 0$ as otherwise there is nothing to show. By the definition of affine margin, there must exist a point a_i such that $\cos \alpha = \frac{w_t}{\|w_t\|} \cdot a_i \leq \rho_A^-$ or equivalently $|\cos \alpha| \geq |\rho_A^-|$. VNG sets w_{t+1} to be the nearest point to the origin on the line joining w_t with a_i . Consider \tilde{w} as the nearest point to the origin on a (dotted) line parallel to a_i through w_t . Note $(\pi/2 - \beta) + \alpha = \pi$ (internal angles of parallel lines). Then, $\|w_{t+1}\| \leq \|\tilde{w}\| = \|w_t\| \cos \beta = \|w_t\| \sin \alpha = \|w_t\| \sqrt{1 - \cos^2 \alpha} \leq \|w_t\| \sqrt{1 - |\rho_A^-|^2}$. \square

Hence, VNG can converge linearly with strict infeasibility of (P), but NP cannot. Nevertheless, NP and VNG can both be seen geometrically as trying to represent the center of circumscribing or inscribing balls (in (P) or (D)) of $\text{conv}(A)$ as a convex combination of input points.

6.2 Summary

In this paper, we advance and unify our understanding of margins through a slew of new results and connections to old ones. First, we point out the correctness of using the affine margin, deriving its relation to the smallest ball enclosing $\text{conv}(A)$, and the largest ball within $\text{conv}(A)$. We proved generalizations of Gordan's theorem, whose statements were conjectured using the preceding geometrical intuition. Using these tools, we then derived interesting variants of Hoffman's theorems that explicitly use affine margins. We ended by

proving that the Perceptron algorithm turns out to be primal-dual, its iterates are margin-maximizers, and the norm of its iterates are margin-approximators.

Right from his seminal introductory paper in the 1950s, Hoffman-like theorems have been used to prove convergence rates and stability of algorithms. Our theorems and also their proof strategies can be very useful in this regard, since such Hoffman-like theorems can be very challenging to conjecture and prove (see [16] for example). Similarly, Gordan’s theorem has been used in a wide array of settings in optimization, giving a precedent for the possible usefulness of our generalization. Lastly, large margin classification is now such an integral machine learning topic, that it seems fundamental that we unify our understanding of the geometrical, analytical and algorithmic ideas behind margins.

Acknowledgements

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A Figures

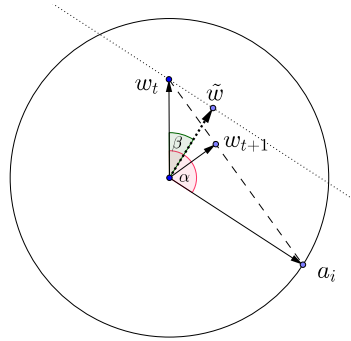


Figure 1: Geometric illustration of a VNG iteration.

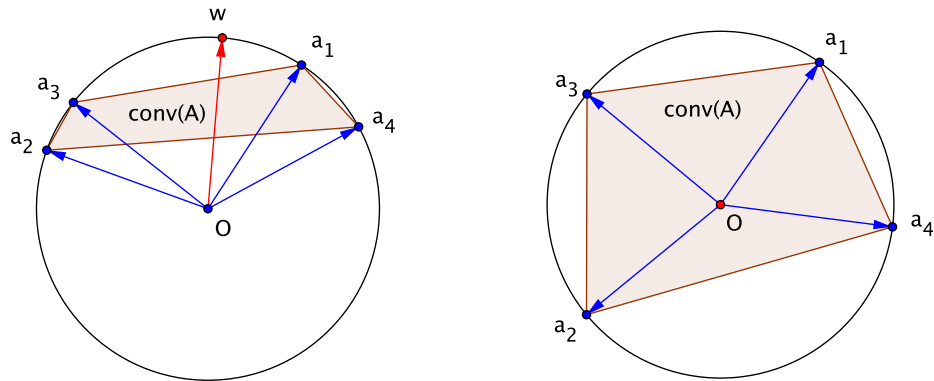


Figure 2: Gordan's Theorem: Either there is a w making an acute angle with all points, or the origin is in their convex hull. (note $\|a_i\| = 1$)

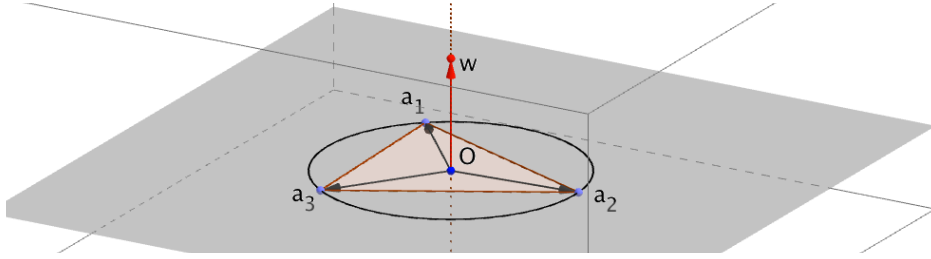


Figure 3: When restricted to $\text{lin}(A)$, the margin is strictly negative. Otherwise, it would be possible to choose w perpendicular to $\text{lin}(A)$, leading to a zero margin.

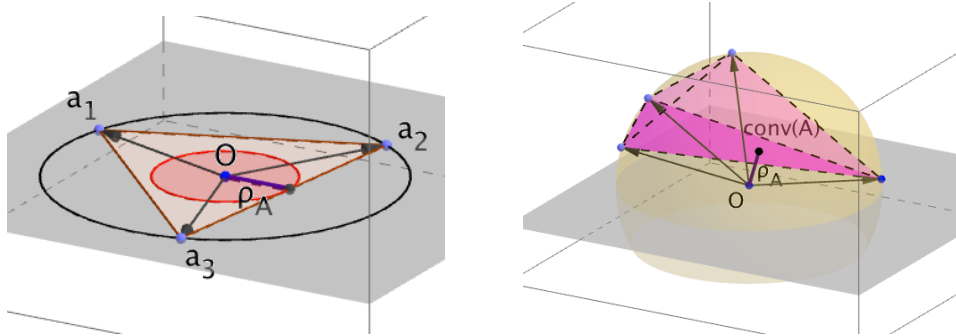


Figure 4: Left: ρ_A^- is the radius of the largest ball centered at origin, inside the relative interior of $\text{conv}(A)$. Right: ρ_A^+ is the distance from origin to $\text{conv}(A)$.